



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 13, 2026 – 08:16 AM EDT

PDB ID : 35WK / pdb_000035wk
Title : Crystal structure of the core catalytic domain of human inositol phosphate multikinase in complex with an inhibitor UNC7844
Authors : Wang, H.
Deposited on : 2026-05-20
Resolution : 1.65 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

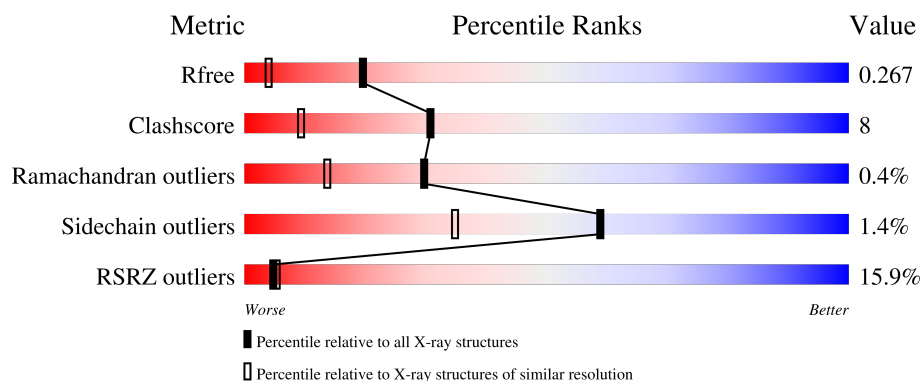
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	261	15% 79% 10% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Inositol polyphosphate multikinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	0	6	0
			1988	1281	331	367	9			

There are 48 discrepancies between the modelled and reference sequences:

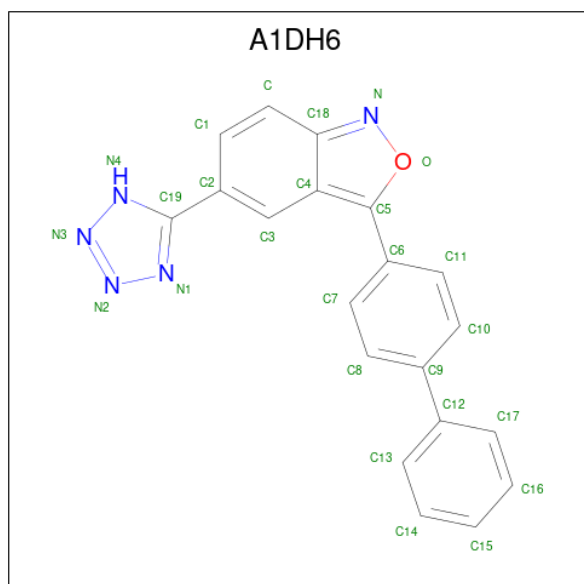
Chain	Residue	Modelled	Actual	Comment	Reference
A	46	GLY	-	expression tag	UNP Q8NFU5
A	47	SER	-	expression tag	UNP Q8NFU5
A	48	PHE	-	expression tag	UNP Q8NFU5
A	49	THR	-	expression tag	UNP Q8NFU5
A	373	GLY	-	expression tag	UNP Q8NFU5
A	374	GLY	-	expression tag	UNP Q8NFU5
A	375	SER	-	expression tag	UNP Q8NFU5
A	376	GLY	-	expression tag	UNP Q8NFU5
A	377	GLY	-	expression tag	UNP Q8NFU5
A	378	GLU	-	expression tag	UNP Q8NFU5
A	379	VAL	-	expression tag	UNP Q8NFU5
A	380	GLU	-	expression tag	UNP Q8NFU5
A	381	VAL	-	expression tag	UNP Q8NFU5
A	382	ARG	-	expression tag	UNP Q8NFU5
A	383	MET	-	expression tag	UNP Q8NFU5
A	384	ILE	-	expression tag	UNP Q8NFU5
A	385	ASP	-	expression tag	UNP Q8NFU5
A	386	PHE	-	expression tag	UNP Q8NFU5
A	387	ALA	-	expression tag	UNP Q8NFU5
A	388	HIS	-	expression tag	UNP Q8NFU5
A	389	VAL	-	expression tag	UNP Q8NFU5
A	390	PHE	-	expression tag	UNP Q8NFU5
A	391	PRO	-	expression tag	UNP Q8NFU5
A	392	SER	-	expression tag	UNP Q8NFU5
A	393	ASN	-	expression tag	UNP Q8NFU5
A	394	THR	-	expression tag	UNP Q8NFU5
A	395	ILE	-	expression tag	UNP Q8NFU5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	396	ASP	-	expression tag	UNP Q8NFU5
A	397	GLU	-	expression tag	UNP Q8NFU5
A	398	GLY	-	expression tag	UNP Q8NFU5
A	399	TYR	-	expression tag	UNP Q8NFU5
A	400	VAL	-	expression tag	UNP Q8NFU5
A	401	TYR	-	expression tag	UNP Q8NFU5
A	402	GLY	-	expression tag	UNP Q8NFU5
A	403	LEU	-	expression tag	UNP Q8NFU5
A	404	LYS	-	expression tag	UNP Q8NFU5
A	405	HIS	-	expression tag	UNP Q8NFU5
A	406	LEU	-	expression tag	UNP Q8NFU5
A	407	ILE	-	expression tag	UNP Q8NFU5
A	408	SER	-	expression tag	UNP Q8NFU5
A	409	VAL	-	expression tag	UNP Q8NFU5
A	410	LEU	-	expression tag	UNP Q8NFU5
A	411	ARG	-	expression tag	UNP Q8NFU5
A	412	SER	-	expression tag	UNP Q8NFU5
A	413	ILE	-	expression tag	UNP Q8NFU5
A	414	LEU	-	expression tag	UNP Q8NFU5
A	415	ASP	-	expression tag	UNP Q8NFU5
A	416	ASN	-	expression tag	UNP Q8NFU5

- Molecule 2 is (5P)-3-([1,1'-biphenyl]-4-yl)-5-(1H-tetrazol-5-yl)-2,1-benzoxazole (CCD ID: A1DH6) (formula: C₂₀H₁₃N₅O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	5	1		

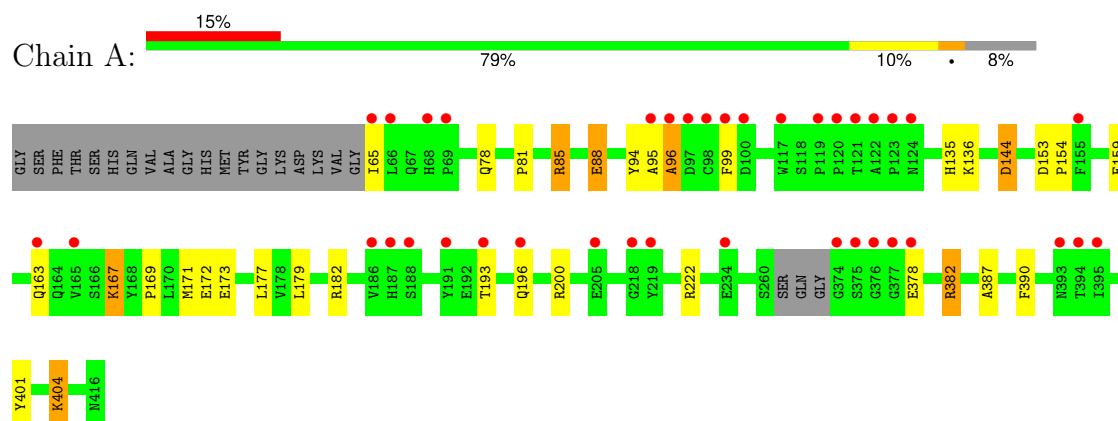
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Inositol polyphosphate multikinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	78.24Å 78.24Å 85.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.38 – 1.65 37.38 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (37.38-1.65) 99.2 (37.38-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.17 (at 1.64Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.216 , 0.256 0.230 , 0.267	Depositor DCC
R_{free} test set	1629 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.5	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2161	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1DH6

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2039	1.13	7/2755 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	PHE	CA-CB-CG	-9.12	104.68	113.80
1	A	88	GLU	CB-CG-CD	7.11	124.68	112.60
1	A	172	GLU	CB-CG-CD	6.59	123.80	112.60
1	A	382	ARG	CG-CD-NE	-6.44	97.82	112.00
1	A	144	ASP	CA-CB-CG	6.18	118.78	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	222	ARG	Sidechain
1	A	382	ARG	Sidechain
1	A	85[A]	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1988	0	1950	33	1
2	A	26	0	0	0	0
3	A	147	0	0	19	1
All	All	2161	0	1950	33	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 33 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85[A]:ARG:HG2	3:A:657:HOH:O	1.65	0.94
1:A:78:GLN:NE2	3:A:605:HOH:O	2.22	0.72
1:A:85[A]:ARG:HD2	1:A:387:ALA:O	1.88	0.72
1:A:171[B]:MET:HE1	1:A:177:LEU:HB2	1.77	0.66
1:A:95:ALA:O	1:A:96:ALA:CB	2.43	0.66

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85[A]:ARG:NH2	3:A:713:HOH:O[6_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	241/261 (92%)	234 (97%)	6 (2%)	1 (0%)	30 14

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	219/230 (95%)	216 (99%)	3 (1%)	59 35

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	196	GLN
1	A	404	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	216	HIS
1	A	163	GLN
1	A	162	GLN
1	A	164	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1DH6	A	501	-	29,30,30	2.18	9 (31%)	36,42,42	2.10	9 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1DH6	A	501	-	-	0/12/12/12	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1DH6	C6-C5	-5.96	1.38	1.47
2	A	501	A1DH6	C2-C19	-4.86	1.38	1.47
2	A	501	A1DH6	C18-C4	-3.74	1.36	1.43
2	A	501	A1DH6	C-C18	-3.59	1.36	1.40
2	A	501	A1DH6	C9-C12	-2.89	1.42	1.49

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1DH6	C19-N1-N2	5.62	112.08	106.10
2	A	501	A1DH6	N1-N2-N3	-5.29	104.19	110.50
2	A	501	A1DH6	C7-C6-C5	4.75	127.70	120.71
2	A	501	A1DH6	O-C5-C4	-3.65	105.58	108.79
2	A	501	A1DH6	O-C5-C6	2.72	121.19	115.48

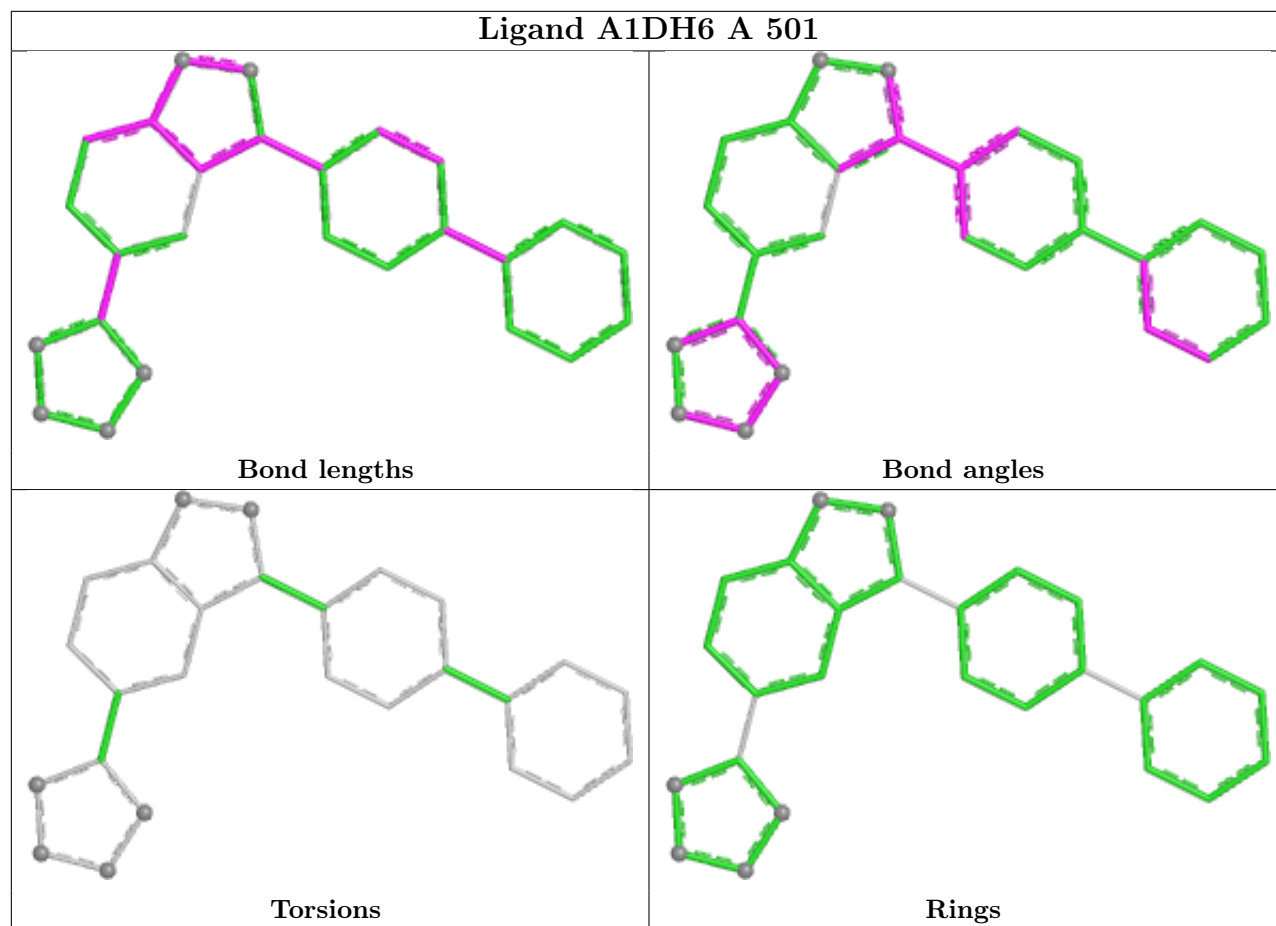
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	239/261 (91%)	0.95	38 (15%) 5 5	3, 24, 49, 75	6 (2%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	99	PHE	6.8
1	A	96	ALA	6.1
1	A	95	ALA	4.6
1	A	122	ALA	4.4
1	A	121	THR	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

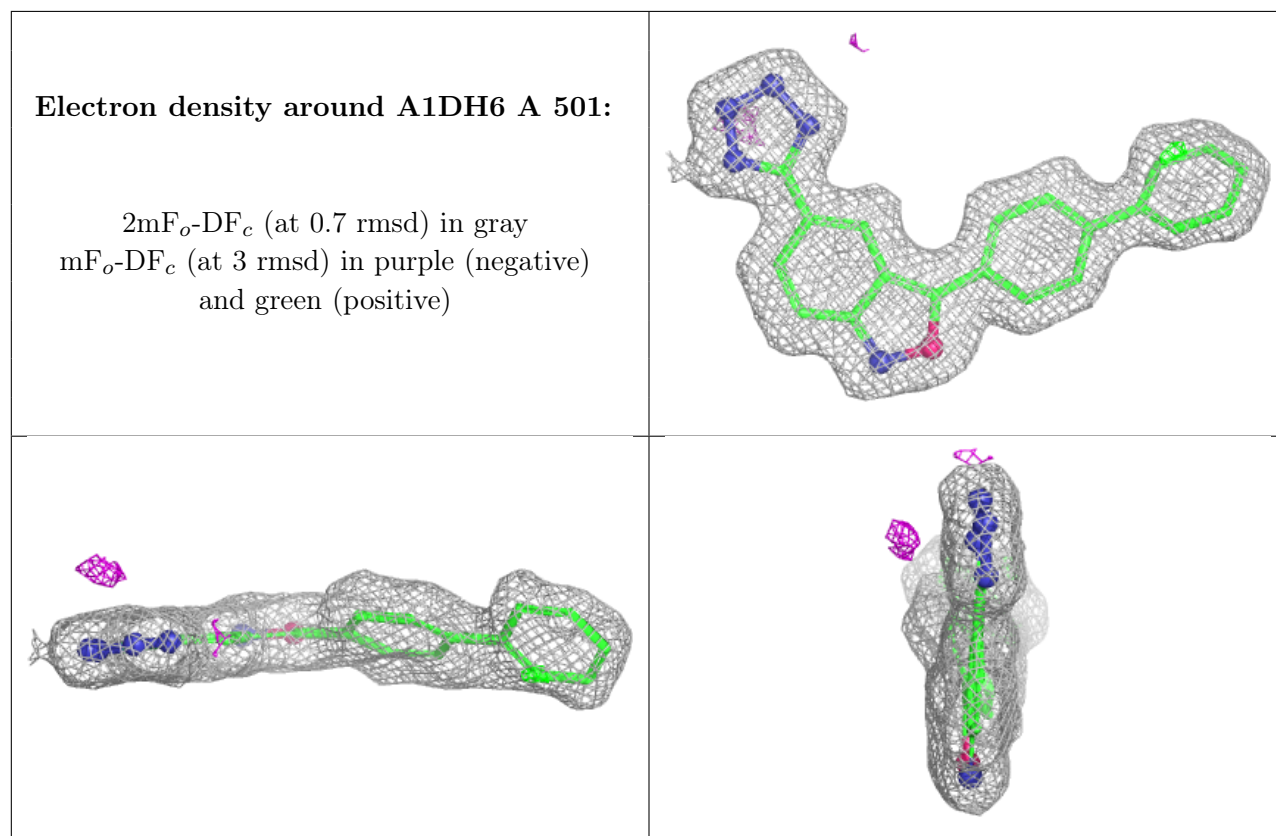
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	A1DH6	A	501	26/26	0.97	0.07	10,13,25,28	0

The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.